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COOPERATIVE SIMULATION TOOL WITH THE ENERGY MANAGEMENT SYSTEM FOR THE STORAGE OF ELECTRICITY SURPLUS THROUGH HYDROGEN

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Abstract. *The INGRID project aims at demonstrating the effective usage of safe, high-density, solid-state hydrogen storage systems for power supply and demand balancing within active power distribution grids with high penetration of intermittent Distributed Generation (Renewable Energy Sources in particular). The INGRID simulator is divided in two main blocks: the first one represents the Energy Management System, the second one includes the Green Energy Storage System (water electrolyzer, hydrogen solid-storage systems and fuel cell) created to simulate the plant. This paper describes the modules of INGRID simulator and the transient responses of the system for a virtual energy management system according to the power prediction of renewable energy sources, hydrogen demand and the power demand of electric vehicles.*

1 INTRODUCTION

The FP7 European co-funded INGRID project tries to contribute to the solution of the instability and non-controllability in the grid by the massive introduction of energy produced by Renewable Energy Sources (RES), proposing a close cooperation with the Distributor System Operator (DSO) towards the balance of the energy demand and supply inside the grid. It combines solid-state high-density hydrogen storage systems with an Energy Management System (EMS). The distributor system operator will take advantage of INGRID both for the absorption of renewable energy sources power and for the provision of ancillary services. In its turn INGRID will move the absorbed energy towards different energy vectors, e.g. hydrogen, or electric vehicle mobility. INGRID concepts will be instantiated into a concrete pilot. The plant will consist of a 39 MWh energy storage facility operating in Puglia region (Troia, Italy).

The main project innovation will consist of combining hydrogen solid-storage systems, where solid magnesium absorbs the hydrogen gas, with smart grid cutting-edge ICT-based active network control technologies for balancing highly variable power supply and demand in a scenario of high penetration of renewable energy sources.

In this project, a specific simulation tool has been developed for predicting and describing INGRID plant behavior before there is any building on the field. The INGRID simulator is divided in several modules with different shared inputs and outputs that create a whole simulation tool. In particular, there are two main blocks: the first one represents the Energy Management System and its inputs/outputs, the second one includes the Green Energy Storage System (GES) created to simulate the plant.

2 DESCRIPTION OF THE COOPERATIVE SIMULATION TOOL WITH THE EMS

The INGRID simulator requires an EMS in order to provide control data for the real plant and make it work and adapt its outputs to the electricity market. The INGRID simulator takes into account two functioning possibilities attending to whether it is connected to a real EMS or to a simulated one. When a real or physical EMS is constructed, it can be connected to the rest of the plant (simulated or real) and work in consequence. While the complete EMS is under development, a simple and functional EMS has been designed in order to provide control inputs to the field simulator, considering a series of estimated parameters: power production, hydrogen market demand and electric vehicles power demand.

Two operation modes are considered. The closed loop refers to the scenario when the hydrogen storage system is connected to a fuel cell to generate electricity. In the case of the open loop, the hydrogen is stored in order to sell it in a container to external customers.

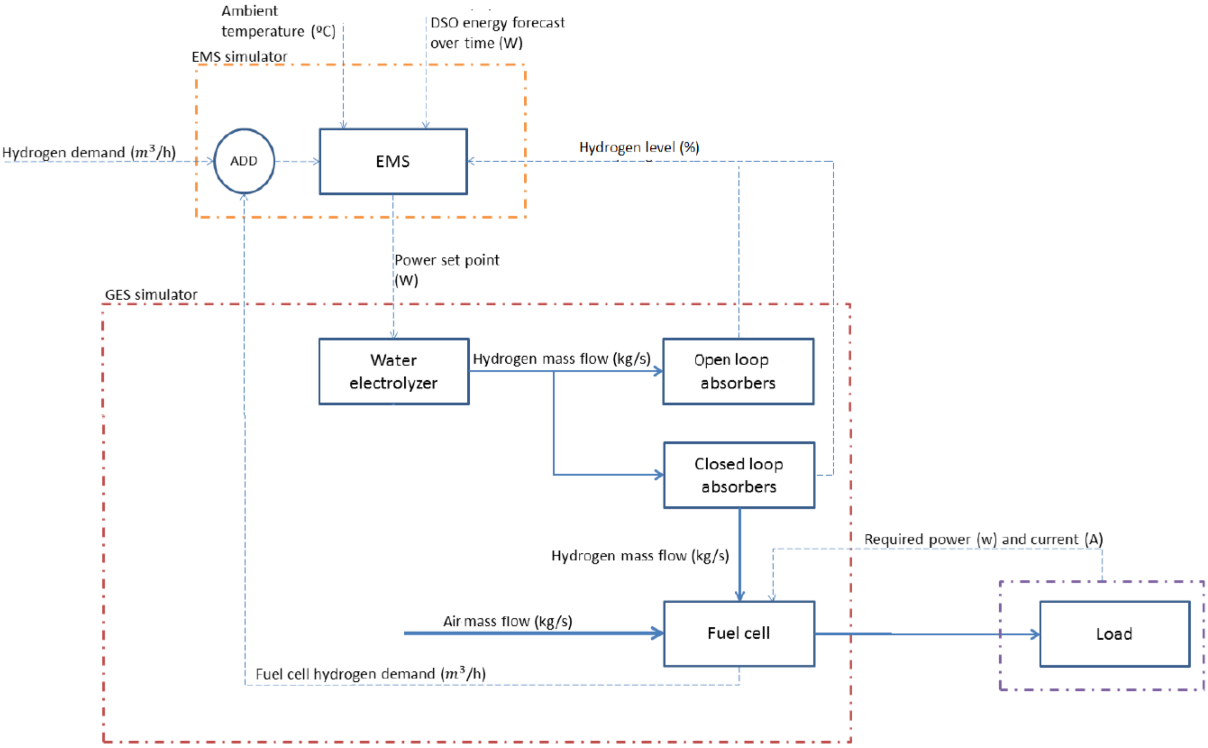

Figure 1. Ingrid plant simulation modules and information flow chart

2.1 The simulated EMS

The aim of the simulated EMS is to verify that the behavior of simulated plant components is faithful to reality. This functional EMS cannot substitute the real one in terms of profit optimization or grid compensation. The logics implemented in this simulated EMS are the following:

1. The hydrogen generated by the water electrolyzer is smartly distributed between the closed loop hydrogen solid storage tanks and the open loop tanks.
2. The operation strategies must fulfil electric vehicles demand, hydrogen demand and grid power demand.
3. Additionally the storage of surplus grid energy should be maximized, according to the profile requested by the grid operator.

There is not a complete optimization module implemented in the simulated EMS; the real EMS should be successively interfaced to the simulated plant for evaluating the accuracy of the energy balancing processes.

The power production estimation module includes both renewable energy sources (modeled according to weather conditions) and other sources (modeled as constant). In this paper wind and photovoltaic plants account for all the power generation.

The estimation of green hydrogen market includes constant and discontinuous demands. Currently, global hydrogen production is 48% from natural gas, 30% from oil, and 18% from coal; water electrolysis accounts for only 4%.

Finally, the estimation of electric vehicles power demand was evaluated according to a model based on statistical arrival curves and estimations for the required energy and the recharging power.

2.2 The INGRID simulation tool

The main components of the green energy storage system are a water electroyzer, a hydrogen solid-storage system and a fuel cell stack.

Modeling of water electrolysis for hydrogen production

In recent years, an increasing number of mathematical models describing water electrolysis process have been developed. Some of these models have been incorporated into simulation programs, which can be used for the optimization and dimensioning of hydrogen energy systems. In the INGRID simulation tool the electrode kinetics of an electrolyzer cell can be mathematically modeled using empirical current-voltage relationships. The current –voltage relationship (the polarization curve) can be represented as a sum of linear, logarithmic and exponential functions.

The balance of energy applied to the system is as follows:

$$V = E_0 + r \cdot I + s \cdot \ln(I) + m \cdot \exp(n \cdot I), \tag{1}$$

$$r = r_a + r_b \cdot T \,, \tag{2}$$

$$s = s_a + s_b \cdot T \,, \tag{3}$$

$$m = m_a \cdot \exp\left(m_b \cdot T\right), \tag{4}$$

where "E_0" is the theoretical potential , "I" is the current, "T" is the operational temperature, "r_a", "r_b", "s_a", "s_b", "m_a", "m_b" and "n" are empirical coefficients that can be numerically calculated using non-linear regression techniques.

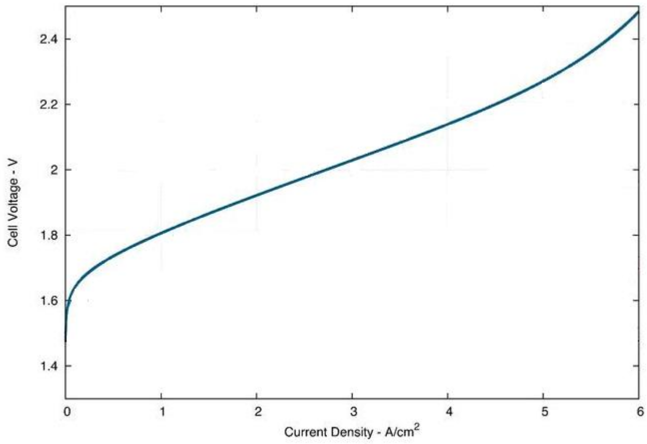

Figure 2. Polarization curve for an electrolyzer cell

The temperature of the electrolyte, which affects the polarization curve and the Faraday efficiency, can be estimated using simple or more complex thermal models. The overall thermal energy balance on the electrolyzer could be expressed by the linear, first order, non-homogeneous differential equation,

$$\frac{dT}{dt} + d_a \cdot T - d_b = 0 \,, \tag{5}$$

which leads to the following solution:

$$T = \left(T_0 - \frac{d_b}{d_a} \right) \cdot e^{-d_a \cdot t} + \frac{d_b}{d_a} \,, \tag{6}$$

where "T_0" is the temperature of cell at initial conditions, "d_a", an empirical parameter that depends on the characteristic of cell and 'd_b' depends on ambient temperature. The temperature "T" of the electrolyte is calculated by using methods of successive substitution.

Modeling of hydrogen solid-storage systems

The hydrogen solid-storage systems developed for the INGRID project are based on metal hydride. The magnesium hydride (MgH_2) was chosen for mass storage because it offers a totally reversible storage. The hydrogen can be absorbed and stored at typical electrolyzer outlet pressure and later hydrogen can be reversibly desorbed at pressure typically adopted into fuel cells and H_2 gas turbines with no intermediate compression stage. Using different temperatures and low pressures, hydrogen is either absorbed or desorbed by the metal.

The tank is connected via a valve to the constant pressure water electrolyzer output. Once the valve is opened, the hydrogen enters the tank and flows through the porous metallic medium. The exothermic absorption process starts and the heat is removed by a cooling fluid in order to get a constant temperature.

The filling kinetics depends on equilibrium relationships between the equilibrium pressure, the ratio of hydrogen to magnesium mass and the temperature. The equilibrium curves are similar to those shown in the next figure.

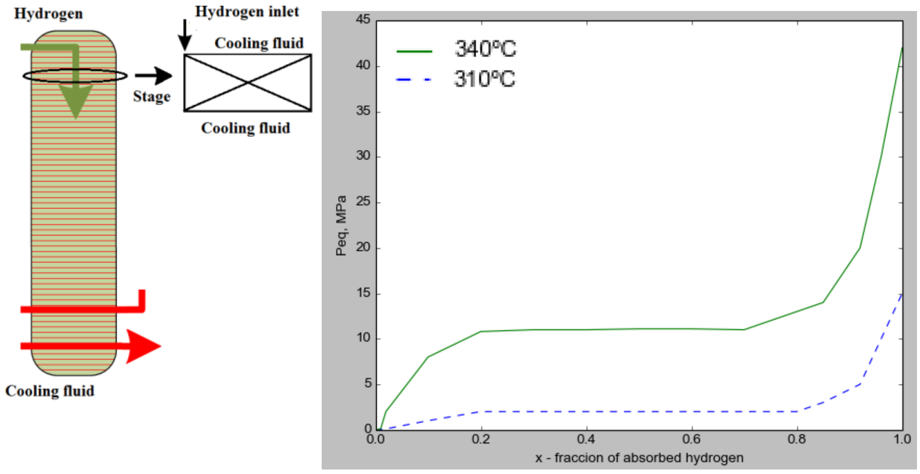

Figure 3. Pressure H_2 weight % - Temperature equilibrium diagram by each stage

The equilibrium relationship is similar to the Langmuir-Freundlich isotherm,

$$x = \frac{b_c \cdot P_{eq}^{\frac{1}{c}}}{1 + b_c \cdot P_{eq}^{\frac{1}{c}}}, \tag{7}$$

$$x = \frac{q}{q_m}, \tag{8}$$

where “P_{eq}“ is the equilibrium pressure for a temperature, “q” is the fraction mass and “q_m” is the equilibrium fraction mass of hydrogen in magnesium.

The kinetics of absorption is defined by the following relationship, according to absorption speed and the balance mass,

$$\frac{dx}{dt} = \frac{C_a}{(1-\varepsilon)} \cdot (1-x) \cdot \exp\left(-\frac{E_a}{R \cdot T}\right) \cdot \ln\left(\frac{P}{P_{eq}}\right), \tag{9}$$

where “C_a” is a constant time, “ε” is the porosity of solid, “E_a”, is the activation energy of the reaction “R”, is the ideal gas constant and “P” is the gas pressure.

On the other hand, the movement of the fluid is given by Darcy law. The continuity equation including the absorption of hydrogen can be expressed as:

$$\varepsilon \cdot \frac{d\rho_{H2}}{dt} = \Delta\rho \cdot (1-\varepsilon) \cdot \frac{dx}{dt}, \tag{10}$$

where “ρ_{H2}“ is the hydrogen density and “$\Delta\rho$“ is the fictitious increase of density of the metal owning to the hydrogenation process. Typically its value is 54 kg/m^3.

In isotherm conditions an approximation to evaluate the kinetics of absorption is given by the next equation,

$$\frac{dx}{dt} = \frac{3 \cdot k}{2} \cdot \frac{(1-x)^{\frac{2}{3}}}{1-(1-x)^{\frac{1}{3}}} \Rightarrow x = 1 - \left(1 - \sqrt{k \cdot t}\right)^3, \tag{11}$$

$$k = k_0 \cdot \left(\frac{P - P_{eq}}{P_{eq}}\right) \cdot \exp\left(\frac{-E_a}{R \cdot T}\right), \tag{12}$$

where k_0 is a specific constant for the absorbent solid, $8 \cdot 10^{-6}$ and T, 613 K.

The variation of the energy in the different steps is evaluated by means of energy balances, where the cooling fluid removes the heat of the exothermic reaction of hydrogen absorption by magnesium. When hydrogen is absorbed and reacts with magnesium to form MgH_2, this heat can be stored, evacuated to be used elsewhere or lost. On the opposite, the reaction of hydrogen desorption by magnesium is an endothermic heat consuming process. This energy can be provided by the heat stored during the absorption reaction or by external components such as electrical heating. In the case of the closed loop the heat is stored as latent heat by means of a cooling fluid. This way it is possible to heat the MgH_2 for desorption process when the fuel cell needs hydrogen. The mathematical model is identical in the case of desorption, considering other equilibrium conditions (11 bar and 340ºC for absorption and 2 bar and 310ºC for desorption).

The process of storage needs different heat levels for different steps of the process as it is shown in next table,

Nº	Step	Notes
1	Ramp-up	System is heated up to the set-point temperature supplying heat (Q_H).
2	Stand-by	To maintain the thermal losses (Q_M)
3	Absorption of hydrogen	To evacuate the heat produced by the chemical reaction (Q_R)
4	Desorption of hydrogen	System is heated up by the endothermic chemical reaction (Q_{ER})
5	Road transportation	The temperature will decrease slowly because the thermal losses are not compensated by electric heaters

Table 1. Steps of the system heating

Modeling of hydrogen fuel cell

In order to produce energy from hydrogen, a fuel cell is necessary. In the INGRID plant, this fuel cell will use the hydrogen of the closed loop tanks.

Fuel cells are classified by the type of electrolyte used in the cells and include: proton exchange membrane (polymer) electrolyte fuel cell (PEM), alkaline fuel cell (AFC), phosphoric acid fuel cell (PAFC), molten carbonate fuel cell (MCPC) and solid oxide fuel cell (SOFC). In the simulator, the fuel cell is modeled as a generic Polymer Electrolyte Membrane fuel cell (PEM), since that's the technology to be used in the INGRID plant.

Depending on the current drawn, the fuel cell converts hydrogen and thereby generates voltage as a function of current. The equations used depend on the empirical form of the fuel cell model. The polarization curve of the fuel cell can be divided into three regions: the activation overvoltage region, the ohmic overvoltage region and the thermodynamic overvoltage region. This curve can be represented by a sum of linear, logarithmic and exponential functions.

The considered model is similar to the electrolyzer model where the balance of energy applied to the system is as follows,

$$V = E_0 + rfc \cdot I + sfc \cdot \ln(I) + mfc \cdot \exp(nfc \cdot I), \quad (13)$$

$$E_0 = 1.299 - 8.5 \cdot 10^{-4} \cdot (T - 25) + 4.3085 \cdot 10^{-5} \cdot (T + 273.15) \cdot (\ln(P_{H2}) + 0.5 \cdot \ln(P_{O2})) \quad (14)$$

$$rfc = rfc_a + rfc_b \cdot T, \quad (15)$$

$$sfc = sfc_a + sfc_b \cdot T, \quad (16)$$

$$mfc = mfc_a \cdot \exp(mfc_b \cdot T), \quad (17)$$

where "E_0" is the theoretical potential , "I" is the current, "T" is the operational temperature, "P_{H2}", "P_{O2}"are the effective partial pressure for hydrogen and oxygen, "rfc_a", "rfc_b", "sfc_a", "sfc_b", "mfc_a", "mfc_b" and "nfc" are empirical coefficients that can be numerically calculated using non-linear regression techniques.

The overall thermal energy balance on the fuel cell could be expressed by a linear, first order, non-homogeneous differential equation.

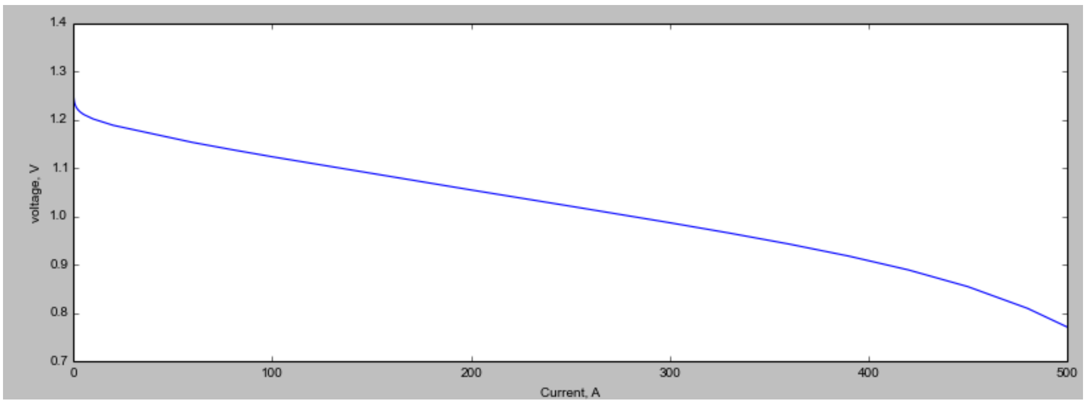

Figure 4. Polarization curves for a fuel cell

2.3 Communications between the INGRID simulation tool and EMS

The EMS will receive information from external sources as the DSO and from the INGRID plant.

The GES module of the INGRID simulation tool is going to be integrated with the real EMS of the INGRID system. The idea is that the real EMS can be alternatively connected either to the simulator or to the real devices, being the simulator an adequate tool to fine tune the EMS and analyze its behavior under different operative scenarios.

Regarding the INGRID communication architecture, a client/server topology is implemented so that the EMS can access and control all the operating parameters. All the devices use the same communication channel, the servers listen and the clients send information when the channel is free.

The EMS could send set points through OLE for Process Control (OPC) over TCP/IP considering the state of GES and the grid requirements of electrical power.

3 SIMULATION RESULTS

The intention of the INGRID simulation tool is to integrate the water electrolyzer, the hydrogen solid-store system and the fuel cell models with the real or virtual EMS that provides control set-points. The simulation tool has been developed in order to foresee how the INGRID plant will evolve during the desired timespan. The tool was programmed in Python and it is possible to define the configuration of hydrogen storage tanks for both the open and the closed loops.

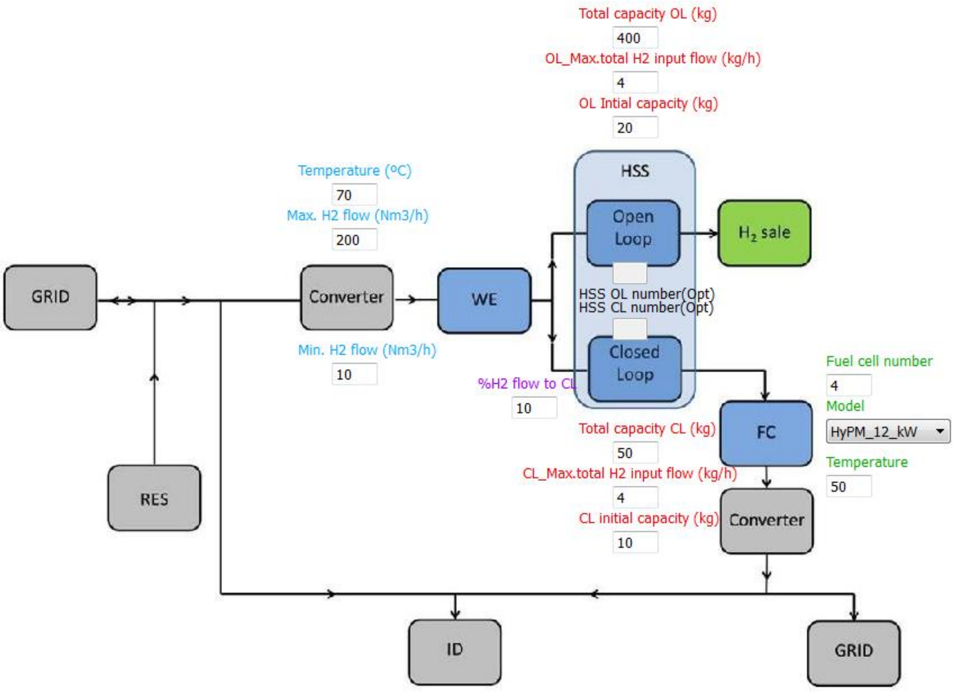

Figure 5. The INGRID simulation tool configuration

After defining hydrogen storage system properties and boundary conditions, the simulated EMS can be executed in order to obtain a control signal to drive the plant simulation. Once this step has been completed, the simulation process can be started using the button created for that purpose.

Next figure shows the estimation of surplus power production and the storage of energy when the INGRID plant is operating during 24 hours. The simulator receives set points from the EMS indicating the required surplus power production to be stored. According to the hydrogen demand and electric vehicle demand curves, the EMS operates the water electrolizer and the fuel cell in order to fulfil the corresponding requirements.

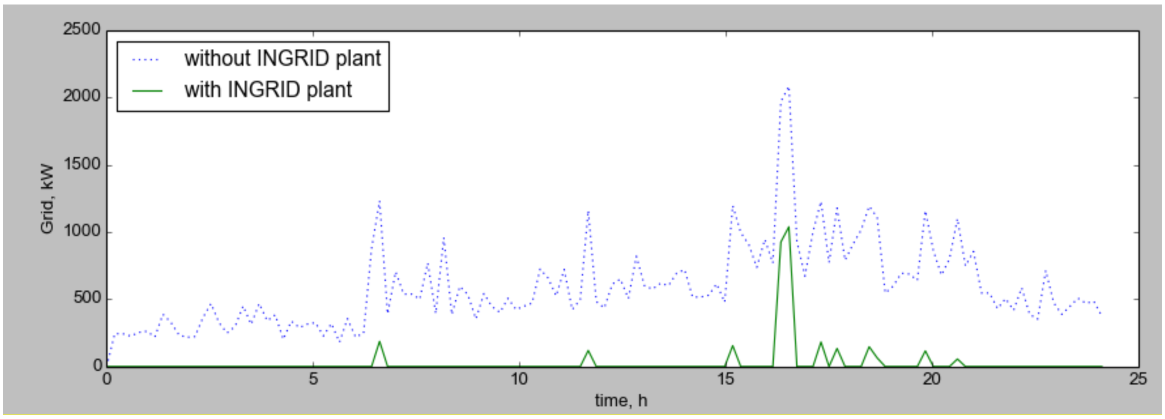

Figure 6. Surplus power production with and without INGRID plant

The behavior of the water electrolyzer is given by its mathematical model and the power set-point provided by the simulated EMS. Next figure shows the time evolution of the water electrolyzer.

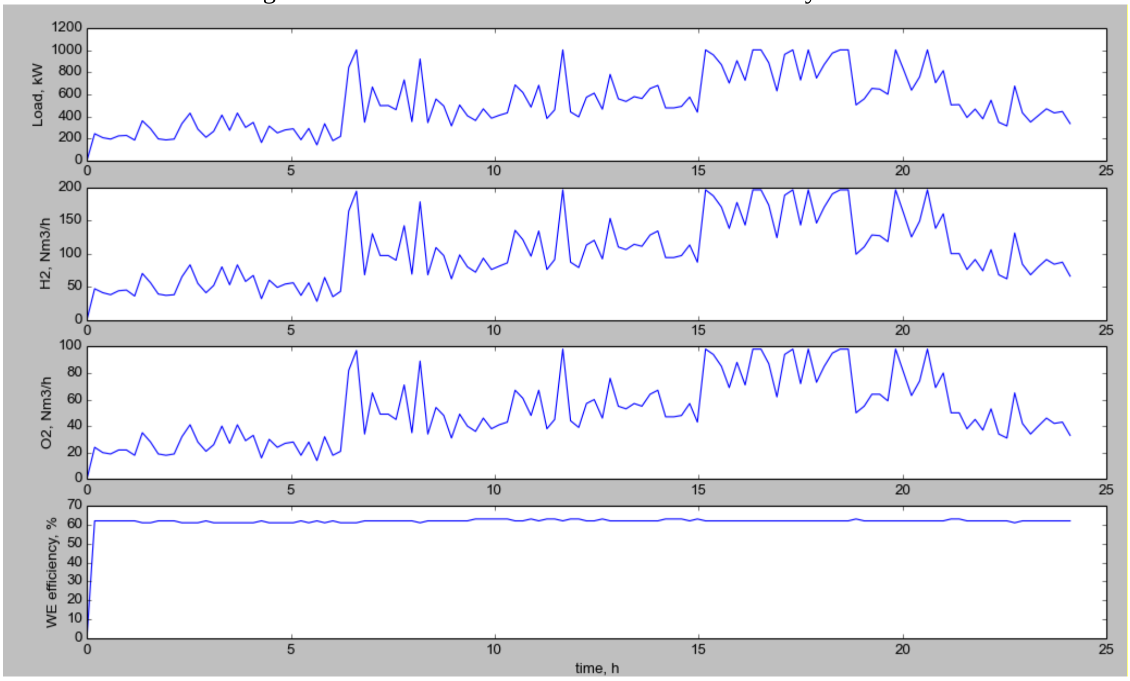

Figure 7. The water electrolyzer behavior according to the simulated EMS logic.

The hydrogen is stored in open and closed loop tanks to meet the hydrogen demand and the electric vehicle demand. Next figure shows the distribution between both systems. Closed loop hydrogen tanks are discharged while the fuel cell generates energy and they are filled when the water electrolyzer operates.

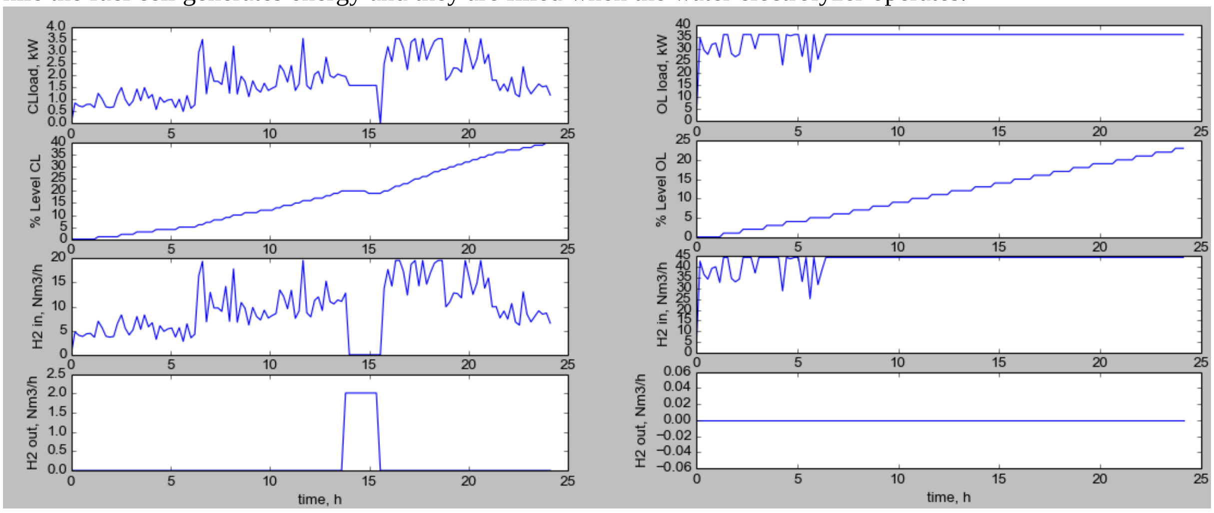

Figure 8. Tank level measured in and in percentage, in closed (left) and open (right) loop, considering energy balance.

In this example, the electric vehicle demand is given by an electric vehicle that needs to recharge its battery.

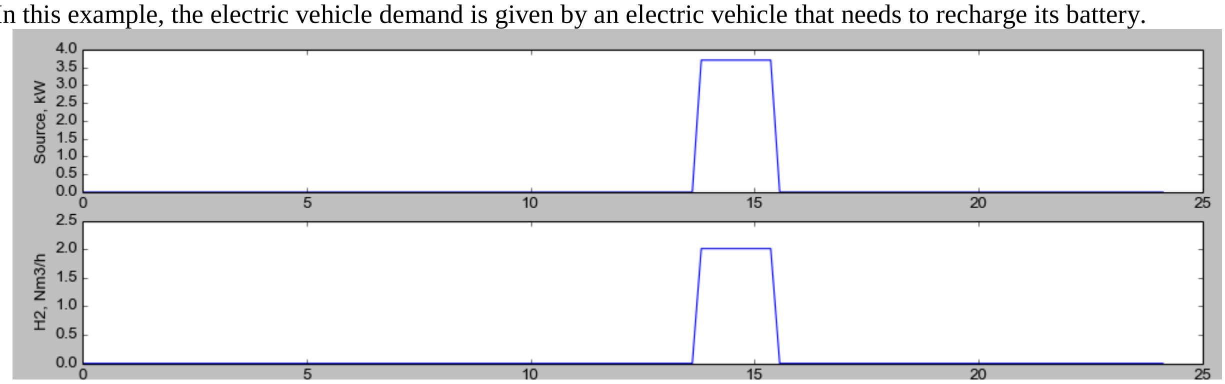

Figure 9. Fuel cell dynamics for one electric vehicle power demand.

4 CONCLUSIONS

This work describes the models for a water electrolyzer, hydrogen solid-storage systems and a fuel cell included in the INGRID simulation tool in cooperation with an EMS. The EMS establishes the power set-points for the water electrolyzer and the fuel cell based on the surplus power production, the estimation of hydrogen demand and the power demand of electric vehicles. The simulator is thus a key tool to fine tune the EMS and anticipate the INGRID plant behavior under different conditions. According to data provided by several partners of INGRID project, physical plant elements have been modeled. Simulation results have been checked against data obtained by vendors. Anyway, the behavior and performance of INGRID plant components working jointly may differ from those indicated by individual tests. Since there is no data related to the whole plant behavior, further developing time will be essential for data acquisition and simulator tuning.

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